U.S. DEPARTMENT OF ENERGY

DOE Office of Science
Advanced Scientific Computing Research
Applied Mathematics Program

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IFIP Working Conference on Uncertainty Quantification in Scientific Computing
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DOE mission imperatives require simulation & analysis for policy and decision making

Energy: Reducing U.S. reliance on foreign energy sources and reducing the carbon footprint of energy production

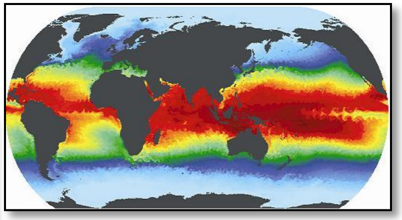
- Reducing time and cost of reactor design & deployment
- Improving the efficiency of combustion energy sources

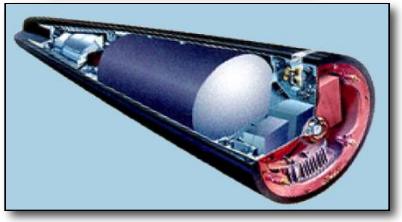
Environment: Understanding, mitigating and adapting to the effects of global warming

- Sea level rise
- Severe weather
- Regional climate change
- Geologic carbon sequestration

National Security: Maintaining a safe, secure and reliable nuclear stockpile

- Stockpile certification
- Predictive scientific challenges
- Real-time evaluation of urban nuclear detonation





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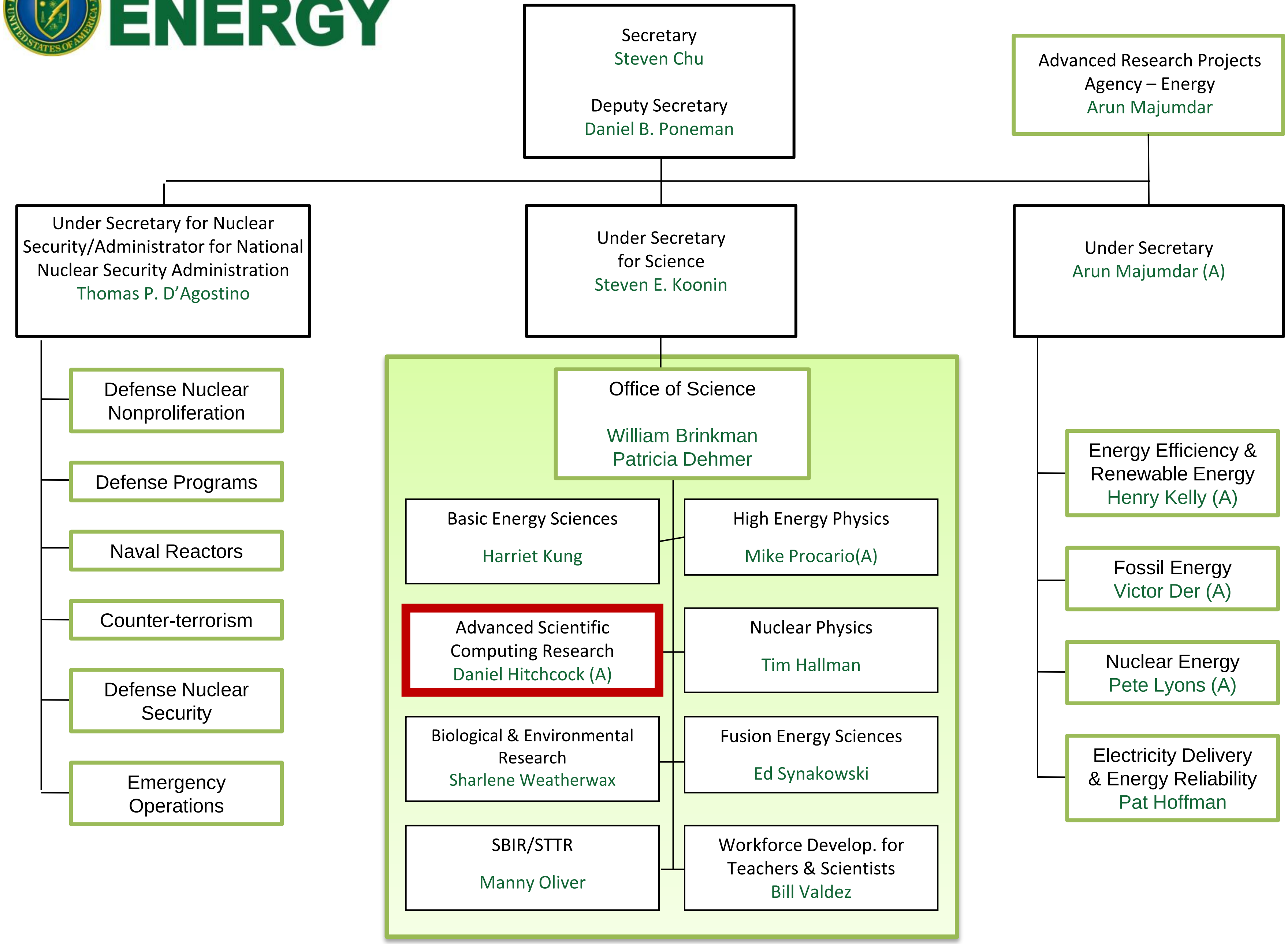

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Advanced Scientific Computing Research (ASCR)

Mission:
Discover, develop, and deploy the computational and networking tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to the Department of Energy.

A particular challenge of this program is fulfilling the science potential of emerging multi-core computing systems and other novel “extreme-scale” computing architectures, which will require significant modifications to today’s tools and techniques.

Advanced Scientific Computing Research Budget

	FY 09	FY 10	FY 11 Request
Applied Mathematics	45,161	44,792	45,450
Computer Science	30,782	46,800	47,400
Computational Partnerships	59,698	53,293	53,297
Next Gen. Networking for Science	14,732	14,321	14,321
High Performance Production Computing (NERSC)	53,497	55,000	56,000
Leadership Computing Facilities (ALCF & OLCF)	116,222	123,168	158,000
High Performance Network Facilities & Testbeds (ESNET)	28,293	29,722	30,000
Research and Evaluation Prototypes	10,387	16,124	10,052
Subtotal, ASCR	358,772	383,220	414,500
All other (SBIR / STTR)	10,048	10,780	11,480
Total, ASCR	368,820	394,000	426,000

Research Division
FY10: ~$159M

Facilities Division
FY10: ~$224M

http://www.science.doe.gov/ascr/Budget/Docs/FY2011CongressionalBudget.pdf

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ASCR and the Path to Exascale Computing

"The emergence of new hardware architectures precludes the option of just waiting for faster machines and then porting existing codes to them. The algorithms and software in those codes must be re-worked." Conclusion 5, The Potential Impact of High-End Capability Computing on Four Illustrative Fields of Science and Engineering, National Research Council, 2008

Goal: Advance the Department's Science, Energy and National Security Missions through modeling and simulation at the extreme scale by the end of the decade

- Provide up to 1,000x more powerful computing resources to
  - Advance scientific frontiers
  - Fully understand National & societal problems, their consequences, solutions and guide policy decisions
- Integrated R&D project with software, hardware and application software
- Broad community participation from universities, labs and industry such as computer vendors and chip manufacturers
- Support competitive research track
- SC and NNSA partner
- Coordinated with HPC efforts supported by DoD, DARPA, and NSF
- Integrated treatment of Intellectual Property

UQ within DOE Office of Science

- Scientific Challenges workshops
- Applied Mathematics program
- SciDAC Institutes
- Co-Design Centers
- Science Application Partnerships

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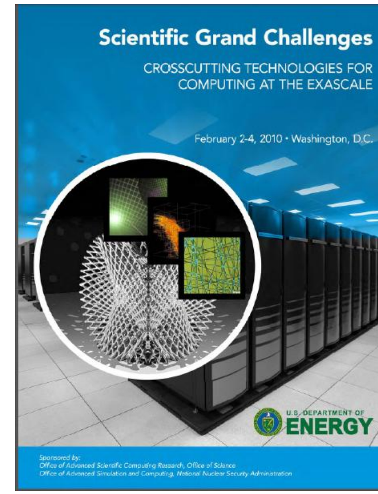
Scientific Challenges Workshops

Scientific Grand Challenges workshops

10 workshops from Feb 2008 – Feb 2010

http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/grand-challenges

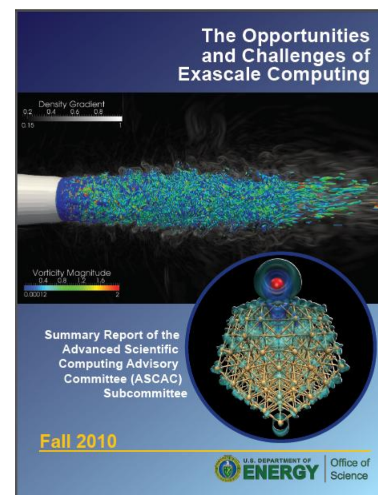


Scientific Grand Challenges: Crosscutting Technologies for Computing at the Exascale

http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Crosscutting_grand_challenges.pdf (pp. 41-46)

UQ promises to become more important as high-end computational power increases for the following reasons:

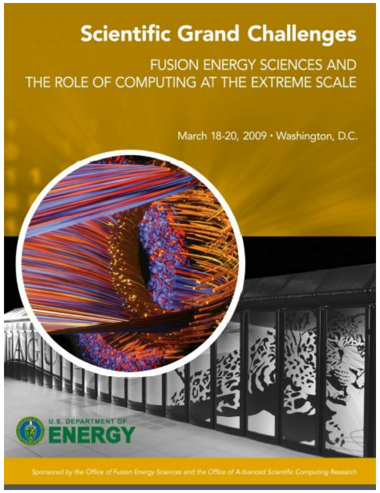
- The scale of computation required to conduct systematic UQ analysis for complex systems will become available
- There will be increasing ability to use computation to access complex physical systems that are progressively more difficult to understand through physical intuition or experiment.
- Exascale capability promises to increase the ability of computational science and engineering to inform policy and design decisions in situations where substantial resources are involved. The quantified confidence measures that UQ will provide are essential to support these decisions.



Scientific Challenges Workshops: Fusion

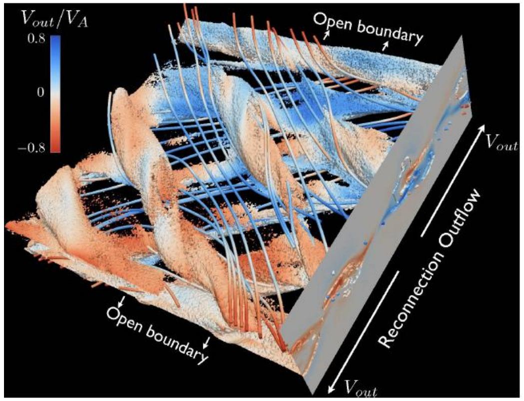
Scientific Grand Challenges: Fusion Energy Science and the Role of Computing at the Extreme Scale

http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Fusion_report.pdf (pp. 103-105)



To achieve predictive simulations with high-fidelity physics for complex fusion devices, a number of advances in numerical methods and computational science are required:

1. Research on efficient error estimation and control, sensitivity analysis, and UQ methods for combined deterministic and stochastic plasma physics models. Hybrid deterministic and probabilistic UQ approaches needed.
2. Probabilistic approaches based on sampling methods (e.g., Monte Carlo) and direct methods (e.g., polynomial chaos).
3. Deterministic UQ tools based on sensitivity and adjoint-based techniques for data, integration, and model error estimation and control.
4. Research on error estimation and UQ for multiphysics, multiscale, multimodel simulations. This includes methods for loosely coupled multiphysics multiscale solvers that would involve data handoffs between multiple codes. Methods for tightly coupled multiphysics and multiscale solution methods are required as well.



Three-dimensional kinetic simulation of magnetic reconnection in a large-scale electron-positron plasma.

Fusion Simulation Program (FSP) Workshop

San Diego, February 8-11, 2011:

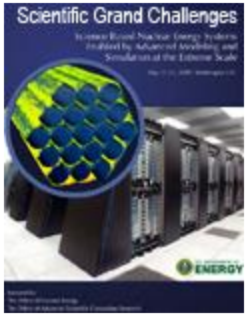
http://www.pppl.gov/fsp/documents/FSP%20Workshop_Summary_Feb2011.pdf

Scientific Challenges Workshops: Nuclear Energy

Science Based Nuclear Energy Systems Enabled by Advanced Modeling and Simulation at the Extreme Scale

http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Sc_nework_shop_report.pdf

(pp. 49-63, 80-82)



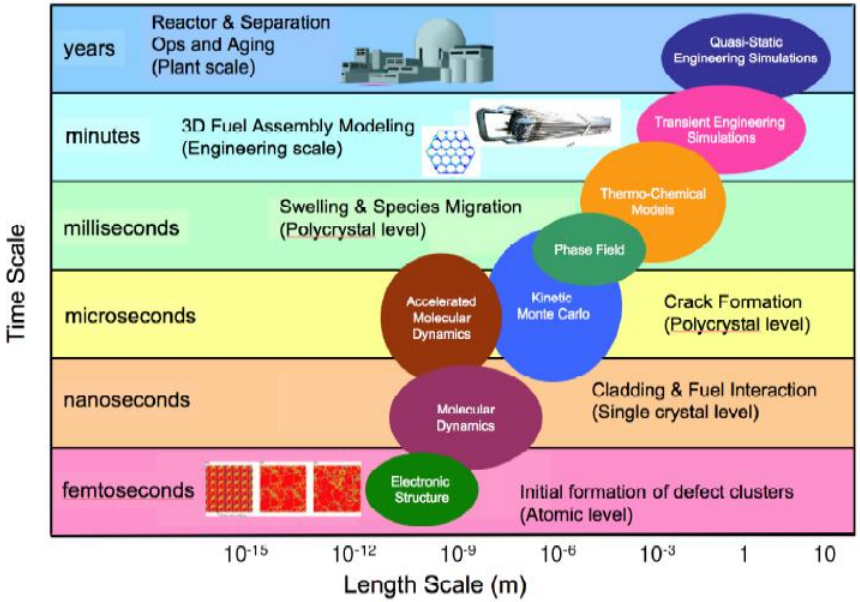
For nuclear energy systems, two main motivations for Verification, Validation and Uncertainty Quantification:

1. Improve the confidence users have in simulations' predictive responses and our understanding of prediction uncertainties in simulations.
2. Scientists must perform V&V / UQ for nuclear energy systems because the US Nuclear Regulatory Commission requires it.

The objective is to predict confidence, using simulation models, best estimate values and the associated uncertainties of complex system attributes, while also accounting for all sources of error and uncertainty.

Report addresses:

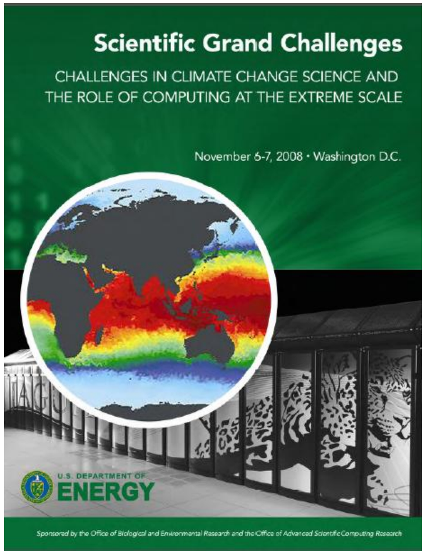
1. Modeling of nuclear energy systems
2. Key elements for Verification and Validation and Uncertainty Quantification
3. Key Issues and Challenges in V&V and UQ
4. Treatment of Nonlinear, Coupled, Multi-Scale Physics Systems
5. Summary of Recommended V&V and UQ Research Priorities



Scientific Challenges Workshops: Climate

Scientific Grand Challenges: Challenges in Climate Change Science and the Role of Computing at the Extreme Scale

http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Climate_report.pdf
(pp. 17-25)



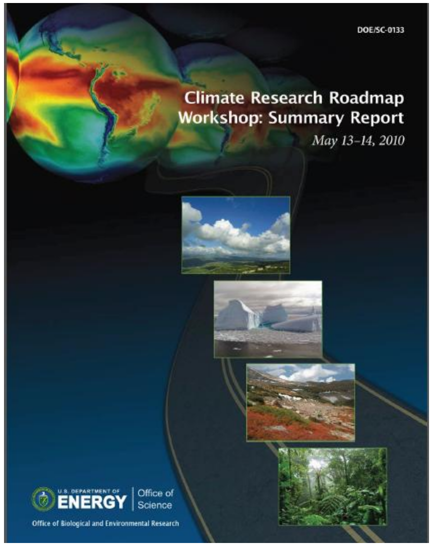
Predictability, initialization, data assimilation and modeling of the climate system present the underlying scientific and computational challenges.

Climate Research Roadmap Workshop (May 2010):

http://science.energy.gov/~/media/ber/pdf/Climate_roadmap_workshop_2010.pdf

Seven overarching recommendations emerged including "Understand and Quantify Uncertainty in Climate Projections"

- An overarching consideration for uncertainty is ensuring that scientific knowledge can be better used to assist decision makers with risk assessment needs.
- Uncertainty needs to be described and quantified in each aspect of process understanding. The resulting understanding needs to be incorporated into models(at all scales) and into the projections of these models.



Applied Math UQ solicitation (FY10)

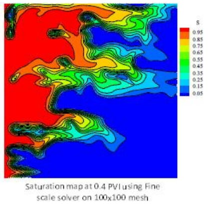
Advancing Uncertainty Quantification (UQ) in Modeling, Simulation, and Analysis of Complex Systems

- Uncertainty quantification refers to the broad range of activities aimed at assessing and improving confidence in simulation. It is important to accurately characterize and quantify the effects of uncertainties and errors on mathematical models and computational algorithms.
- Uncertainty quantification (UQ) broadly refers to the assessment of confidence of simulation predictions based on all available information including:
  - Accuracy of physical measurements;
  - Incomplete understanding of the underlying physical processes;
  - The complexity of coupling different physical processes across large-scale differences;
  - Numerical errors associated with simulations of complex models; and
  - The sensitivity of simulation output to inputs.
- Research in applied mathematics on Uncertainty Quantification in complex systems of interest to the DOE, scalable UQ methods, and UQ relevant to the simulation and analysis of complex systems on high-concurrency, extreme-scale computing architectures.

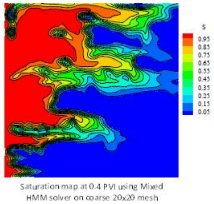
http://science.energy.gov/~/media/ascr/pdf/funding/notices/De_foa_0000315.pdf
http://science.energy.gov/~/media/ascr/pdf/funding/notices/Lab_10_315.pdf

Summary of UQ Awards

1. Modeling and Simulation of High-Dimensional Stochastic Multiscale PDE Systems at the Exascale
   – Guang Lin (PNNL), Nicholas Zabaras (Cornell), and Ioannis Kevrekidis, (Princeton)
2. Advanced Dynamically Adaptive Algorithms for Stochastic Simulations on Extreme Scales
   – Richard Archibald, Ralf Deiterding, and Cory Hauck (ORNL), Dongbin Xiu (Purdue)
3. A High-Performance Embedded Hybrid Methodology for Uncertainty Quantification with Applications
   – Charles Tong (LLNL), Barry Lee (PNNL), Gianluca Iaccarino (Stanford)
4. Enabling Predictive Simulation and UQ of Complex Multiphysics PDE Systems by the Development of Goal-Oriented Variational Sensitivity Analysis and a-Posteriori Error Estimation Methods
   – John Shadid (SNL), Don Estep (CSU), Victor Ginting (UWyoming)
5. Bayesian Uncertainty Quantification in Predictions of Flows in Highly Heterogeneous Media and its Application to CO2 Sequestration
   – Yalchin Efendiev (Texas A&M), Panayot Vassilevski (LLNL)
6. Large-Scale Uncertainty and Error Analysis for Time-Dependent Fluid/Structure interactions in Wind Turbine Applications
   – Michael Eldred, et al (SNL) and Juan Alonso (Stanford)

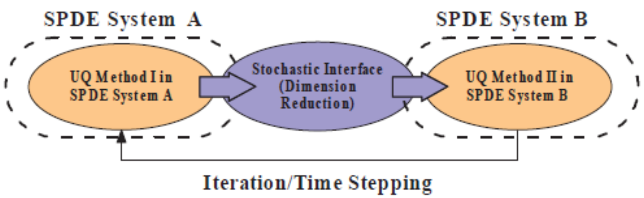


Fine mesh

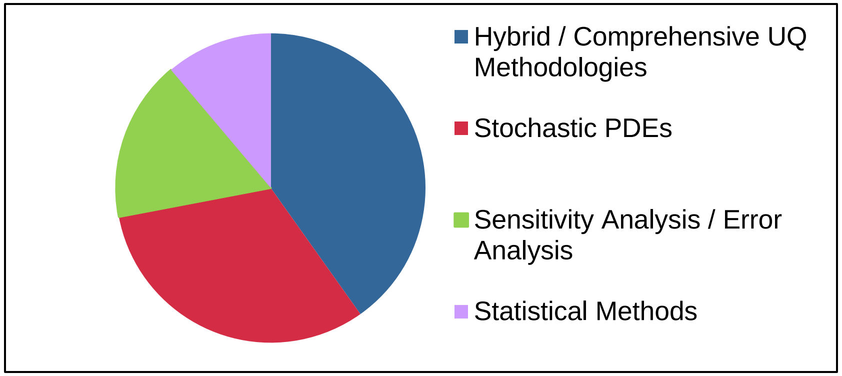


Coarse-graining

Saturation profile of oil-water porous media flow using fine and multiscale coarse-graining solver



Sketch of hybrid UQ method between multi-physics stochastic PDE systems



UQ & Early Career Research Program

- New program started in 2010
- Four Applied Mathematics awardees to date
- Two awards in Uncertainty Quantification
  - Youssef Marzouk, Massachusetts Institute of Technology, "*Predictive Modeling of Complex Physical Systems: New Tools for Uncertainty* " (2010 awardee)
  - Alireza Doostan, University of Colorado Boulder, "*An Enabling Computational Framework for Uncertainty Assimilation and Propagation in Multi-physics Systems: Sparse and Low-rank Techniques*" (2011 awardee)

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Scientific Discovery through Advanced Computing (SciDAC) Institutes

FASTMath – Frameworks, Algorithms, and Scalable Technologies for Mathematics

Director - Lori Diachin, LLNL: Structured & unstructured mesh tools, linear & nonlinear solvers, eigensolvers, particle methods, time integration, differential variational inequalities

SUPER – Institute for Sustained Performance, Energy and Resilience

Director - Robert F. Lucas, USC: Performance engineering, energy efficiency, resilience & optimization

QUEST – Quantification of Uncertainty in Extreme Scale Computations

Director - Habib N. Najm, SNL: Forward uncertainty propagation, reduced stochastic representations, inverse problems, experimental design & model validation, fault tolerance

FASTMath	SUPER	QUEST
Argonne National Laboratory	Argonne National Laboratory	Los Alamos National Laboratory
Lawrence Berkeley National Lab	Lawrence Berkeley National Lab	**Sandia National Laboratories**
Lawrence Livermore National Lab	Lawrence Livermore National Lab	
Sandia National Laboratories	Oak Ridge National Laboratory	
Rensselaer Polytechnic Institute	University of California, San Diego	Johns Hopkins University
	University of Maryland	Massachusetts Institute of Technology
	University of North Carolina	University of Southern California
	University of Oregon	University of Texas at Austin
	University of Utah	
	University of Southern California	
	University of Tennessee, Knoxville	

Three Exascale Co-Design Centers Awarded

Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx)

Director: Timothy Germann (LANL)

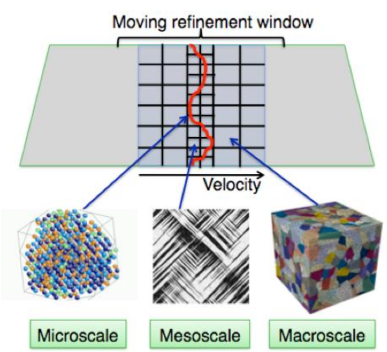
Center for Exascale Simulation of Advanced Reactors (CESAR)

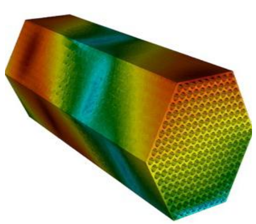
Director: Robert Rosner (ANL)

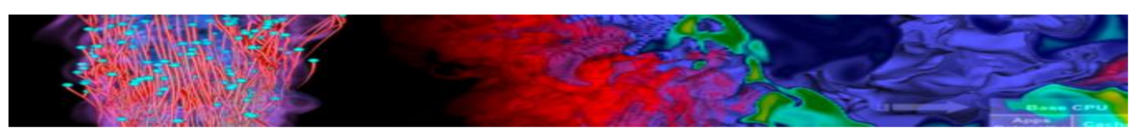
Combustion Exascale Co-Design Center (CECDC)

Director: Jacqueline Chen (SNL)

	ExMatEx (Germann)	CESAR (Rosner)	CECDC (Chen)
National Labs	LANL	ANL	SNL
	LLNL	PNNL	LBNL
	SNL	LANL	LANL
	ORNL	ORNL	ORNL
		LLNL	LLNL
			NREL
University & Industry Partners	Stanford	Studsvik	Stanford
	CalTech	TAMU	GA Tech
		Rice	Rutgers
		U Chicago	UT Austin
		IBM	Utah
		TerraPower	
		General Atomic	
		Areva	







Co-Design Centers & UQ

Exascale Co-design Center for Materials in Extreme Environments

http://exascaleresearch.labworks.org/uploads/dataforms/C_OPH_LANL_ExMatEx_110228.pdf

Scale-bridging algorithms: The science strategy is a UQ-driven adaptive physics refinement in which coarse-scale simulations spawn sub-scale direct numerical simulations as needed.

Center for Exascale Simulation of Advanced Reactors

http://exascaleresearch.labworks.org/ascr2011/index/materials

Uncertainty Quantification: Simulations are predictive only to the extent to which they have been verified, validated, and subjected to detailed error analysis. The optimal strategies of the CESAR project are intimately tied to algorithmic choices for *TRIDENT*, the programming model ultimately chosen, and the nature of the underlying computer architecture and thus are inherently part of the co-design process.

Combustion Exascale Co-Design Center

http://exascaleresearch.labworks.org/uploads/dataforms/C_OPH_SNL_Combustion_110302.pdf

Uncertainty Quantification:

- Investigate data structures and data management approaches needed to integrate UQ into simulation framework.
- Explore different data-staging approaches to facilitate computation of derivative information from time-dependent simulations
- Investigate in situ analytics support needed for integrated UQ
- Explore potential hardware support needed for intrusive UQ algorithms such as polynomial chaos expansions

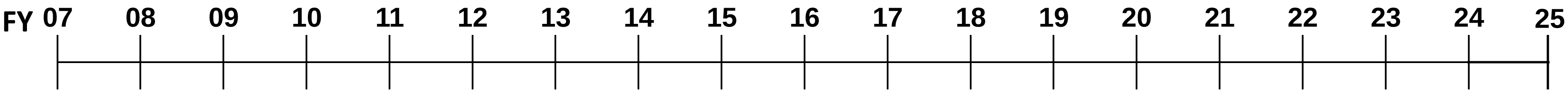
Science Application Partnerships

- Science Applications (http://www.scidac.gov/app_areas.html):
  - Physics: Computational Astrophysics, Quantum Chromodynamics, High Energy Physics, Nuclear Physics and Combustion
  - Climate Modeling and Simulation
  - Groundwater Reactive Transport Modeling and Simulation
  - Fusion Science
  - Computational Biology
  - Materials Science & Chemistry
- Science Application Partnerships (SAPs or Partnerships) offer support for multidisciplinary interaction among application domains, computer science, and applied mathematics. SAPs enable applied mathematics and computer science research to significantly enhance a targeted Science Application project.
- New solicitations starting Summer 2011.

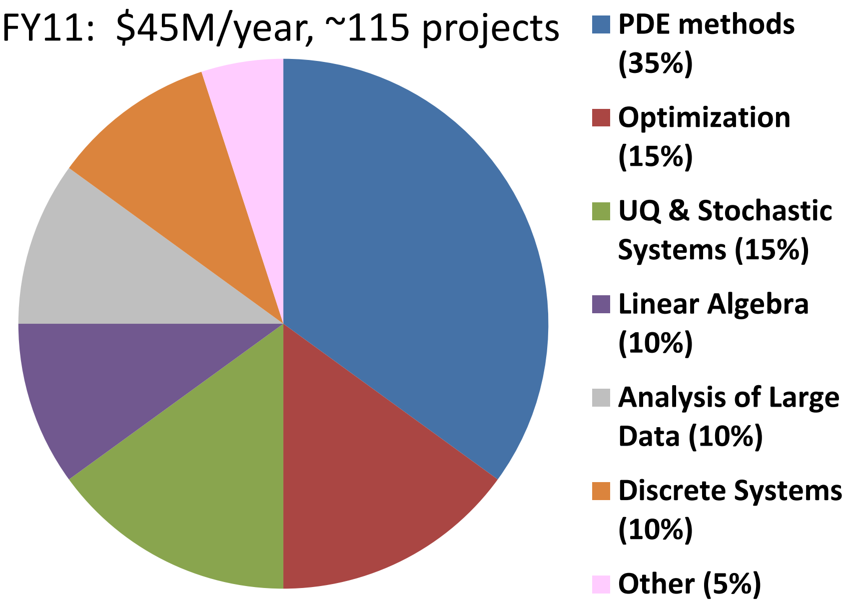
Back to Future …
in Applied Mathematics

Applied Mathematics Future Directions

The DOE Applied Mathematics program supports basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions; develop robust mathematical models, algorithms and numerical software for enabling predictive scientific simulations of DOE-relevant complex systems.



FY11: $45M/year, ~115 projects



Algorithms for predictive science, analysis, and science-based decision support:

- Increase fidelity: develop new multi-scale, multi-physics models
- Uncertainty Quantification and V&V
- Novel analysis algorithms for large data / streaming data
- Solvers and optimization methods with reduced global communication
- Higher-order methods; accuracy, stability of methods that move away from bulk synchronous programming models
- Resilient algorithms
- Rigorous analysis of algorithms for emerging architectures

Multicore:
Here and now

Manycore /
Hybrid
Architectures

Questions, comments, feedback, solutions all graciously accepted.

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